

A LEVEL-SET BASED MODEL OF MEMS FABRICATION PROCESSES AT FEATURE LENGTH SCALES

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Theoretical modeling of the detailed surface chemistry and concomitant surface evolutions during microsystems fabrication processes is recognized as having great potential for improving surface micromachining, SMM process fabrication technologies. For example, there is a clear need to better understand the fundamental factors leading to surface non-uniformities and how to control these effects. The value of modeling in this area has been demonstrated by earlier researchers and advances have been made in developing transport. However, currently available computer codes have not been designed to use efficiently large parallel architectures, nor fully exploit all of the modeling advances that different researchers have made. Thus size and complexity of problems that have been addressed has been limited.

We are developing ChISELS (Chemically Induced Surface Evolution with Level-Sets), a parallel code to model 3-D material depositions and etches at feature scales on patterned wafers at low pressures. The framework in which the ChISELS code is built is based upon the level-set method for modeling evolving interfaces. The level-set method, an implicit interface tracking technique, was chosen for its natural ability to handle changes in topology that frequently occur, for example, when films are grown in high aspect-ratio features in MEMS devices. The hyperbolic partial differential equation that, based on interface velocities determined from the physics of a growth or etch problem, governs the evolution of the level-set function is solved by the semi-Lagrangian method. The semi-Lagrangian method is used here because, (1) it works well for hyperbolic systems without special treatments (e.g. upwinding), (2) time integration is explicit and only interpolation on the grid is required to solve for the level-set function at the next time step, and (3) it is well-suited to the massively parallel computing environments used at Sandia National Laboratories. The meshes used in ChISELS are quad-trees (2-D) and oct-trees (3-D). The quad-trees are constructed such that the grid is refined only in the region of the interface. As the interface evolves, the static mesh is continually reconstructed so that the grid remains fine only around the interface. For parallel computation, the grid is distributed across the processors with each one owning a compact sub-domain. Each time the mesh is refined and coarsened, the load balance across processors is re-evaluated and redistributed so that the load remains evenly balanced regardless of changes in the grid.

From the level-set function, the surface is discretized into linear (planar) elements. A ballistic transport model is employed to solve for the fluxes incident on each of the surface elements. Surface Chemkin is used to model the chemical reactions at each surface element determining the rate of growth of the surface there.

Presented here is a description of the algorithm by which the surface is evolved in process models as well as the transport model and the tools used for modeling chemical reactions and dynamic balancing of computational load in a massively parallel environment. To demonstrate the performance of the ChISELS code, an example is given of the growth in a simple feature of silicon from silane, silicon from chlorosilane and silicon dioxide from tetraethoxysilane (TEOS).